

1,2-Benzenedicarboxylic acid, bis(trimethylsilyl) ester

Other names:

Phthalic acid (tms)

Phthalic acid, 2tms derivative

Inchi:

InChI=1S/C14H22O4Si2/c1-19(2,3)17-13(15)11-9-7-8-10-12(11)14(16)18-20(4,5)6/h7-10

InchiKey:

JUZOFKLPPHUUMC-UHFFFAOYSA-N

Formula:

C14H22O4Si2

SMILES:

C[Si](C)(C)OC(=O)c1ccccc1C(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

310.49

CAS:

2078-22-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.27		Crippen Method
logp	3.670		Crippen Method
rinpol	1675.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1675.00		NIST Webbook

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078220&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/55-626-6/1-2-Benzenedicarboxylic-acid-bis-trimethylsilyl-ester.pdf>

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